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FULL ESTIMATED COST	0.21	0.21

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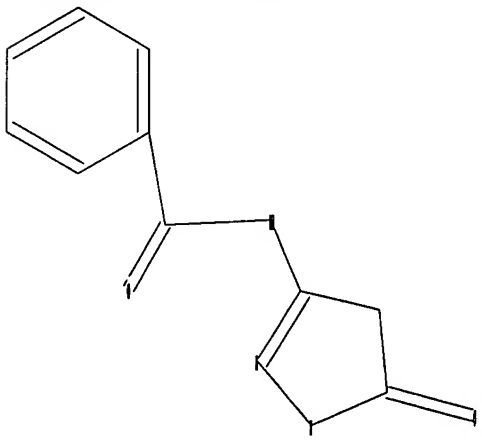
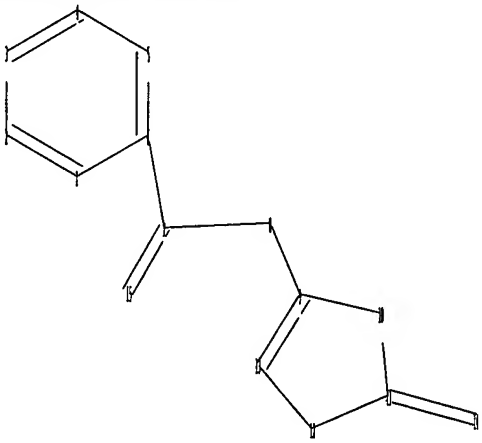




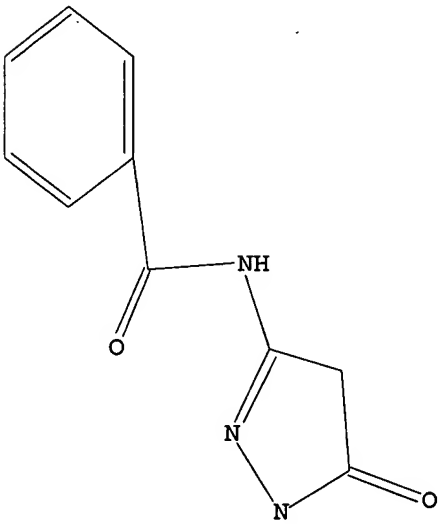
chain nodes :
7 8 14 15
ring nodes :
1 2 3 4 5 6 9 10 11 12 13

chain bonds :
6-7 7-8 7-15 8-9 11-14
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 9-10 9-13 10-11 11-12 12-13
exact/norm bonds :
7-8 7-15 8-9 9-13 11-12 11-14 12-13
exact bonds :
6-7 9-10 10-11
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 : 9 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:CLASS 15:CLASS

L1 STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1
SAMPLE SEARCH INITIATED 10:10:20 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 116 TO ITERATE

100.0% PROCESSED 116 ITERATIONS 50 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

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                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:          1674 TO     2966
PROJECTED ANSWERS:             1265 TO     2415

L2           50 SEA SSS SAM L1

=> s l1 full
FULL SEARCH INITIATED 10:12:40 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -      2436 TO ITERATE

100.0% PROCESSED     2436 ITERATIONS                          1950 ANSWERS
SEARCH TIME: 00.00.05

L3          1950 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                   168.70     168.91

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=> s l3 and barium
          1144 L3
        247945 BARIUM
            12 BARIUMS
        247947 BARIUM
                 (BARIUM OR BARIUMS)
L4           4 L3 AND BARIUM

=> d ibib abs histr tot
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ALL --------- BIB, AB, IND, RE
APPS -------- AI, PRAI
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BIB --------- AN, plus Bibliographic Data and PI table (default)
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CBIB -------- AN, plus Compressed Bibliographic Data
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DMAX -------- MAX, delimited for post-processing
FAM --------- AN, PI and PRAI in table, plus Patent Family data
FBIB -------- AN, BIB, plus Patent FAM
IND --------- Indexing data
IPC --------- International Patent Classifications
MAX --------- ALL, plus Patent FAM, RE
PATS -------- PI, SO
SAM --------- CC, SX, TI, ST, IT
SCAN -------- CC, SX, TI, ST, IT (random display, no answer numbers;
              SCAN must be entered on the same line as the DISPLAY,
              e.g., D SCAN or DISPLAY SCAN)
STD --------- BIB, CLASS

IABS -------- ABS, indented with text labels
IALL -------- ALL, indented with text labels
IBIB -------- BIB, indented with text labels
IMAX -------- MAX, indented with text labels
ISTD -------- STD, indented with text labels

OBIB -------- AN, plus Bibliographic Data (original)
OIBIB ------- OBIB, indented with text labels

SBIB -------- BIB, no citations
SIBIB ------- IBIB, no citations

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HITIND ------ IC, ICA, ICI, NCL, CC and index field (ST and IT)
              containing hit terms
HITRN ------- HIT RN and its text modification
HITSTR ------ HIT RN, its text modification, its CA index name, and
              its structure diagram
HITSEQ ------ HIT RN, its text modification, its CA index name, its
              structure diagram, plus NTE and SEQ fields
FHITSTR ----- First HIT RN, its text modification, its CA index name, and
              its structure diagram
FHITSEQ ----- First HIT RN, its text modification, its CA index name, its
              structure diagram, plus NTE and SEQ fields
KWIC -------- Hit term plus 20 words on either side
OCC --------- Number of occurrence of hit term and field in which it occurs

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information will be displayed in the same order as the format
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=> d ibib abs hitstr tot
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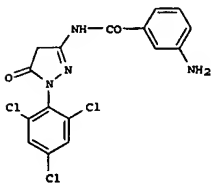
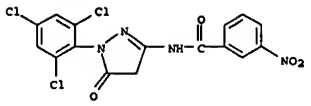
L4 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:495149 CAPLUS
DOCUMENT NUMBER: 144:232961
TITLE: Synthesis of 3-(3''-aminobenzoylamido)-1-(2',4',6'-trichlorophenyl)pyrazol-5-one, an intermediate in the synthesis of the purple component of color photographic materials
AUTHOR(S): Yutilov, Yu. M.; Smolyar, N. N.; Minkina, L. V.
CORPORATE SOURCE: Litvinenko Institute of Physical Organic and Coal Chemistry, National Academy of Sciences of Ukraine, Donetsk, Ukraine
SOURCE: Russian Journal of Applied Chemistry (2005), 78(2), 278-280
CODEN: RJACEO; ISSN: 1070-4272
PUBLISHER: Pleiades Publishing, Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



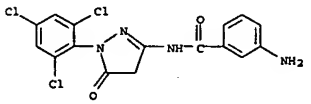
I

AB Catalytic reduction of 3-(3''-nitrobenzoylamido)-1-(2',4',6'-trichlorophenyl)pyrazol-5-one with hydrogen and hydrazine hydrate to 3-(3''-aminobenzoylamido)-1-(2',4',6'-trichlorophenyl)pyrazol-5-one (I), the key intermediate in the synthesis of the purple component of color photog. and motion picture materials, was studied.
IT 63134-25-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of (aminobenzoylamido)(trichlorophenyl)pyrazolone via reduction of
its nitrobenzoyl analog by hydrogen or hydrazine catalyzed by Group 10 metal catalysts)
RN 63134-25-8 CAPLUS
CN Benzamide, N-(4,5-dihydro-5-oxo-1-(2,4,6-trichlorophenyl)-1H-pyrazol-3-yl]-3-nitro- (9CI) (CA INDEX NAME)

L4 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



IT 40567-18-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of (aminobenzoylamido)(trichlorophenyl)pyrazolone via reduction of
its nitrobenzoyl analog by hydrogen or hydrazine catalyzed by Group 10 metal catalysts)
RN 40567-18-8 CAPLUS
CN Benzamide, 3-amino-N-[4,5-dihydro-5-oxo-1-(2,4,6-trichlorophenyl)-1H-pyrazol-3-yl]- (9CI) (CA INDEX NAME)



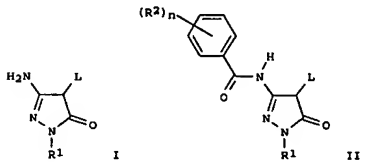
REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L4 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:819915 CAPLUS
DOCUMENT NUMBER: 141:296015
TITLE: Preparation of 3-amino-4-substituted-5-pyrazolones
INVENTOR(S): Mori, Hideto
PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 14 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2004277331	A2	20041007	JP 2003-70179	20030314
US 2004204589	A1	20041014	US 2004-797038	20040311

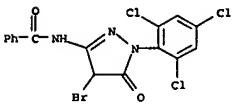
PRIORITY APPLN. INFO.: JP 2003-70179 A 20030314

OTHER SOURCE(S): CASREACT 141:296015; MARPAT 141:296015
GI

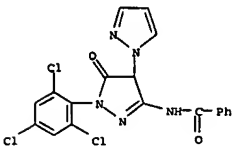


AB The pyrazolones I (R1 = alkyl, aryl; L = thiocyano, aryloxy, alkoxy, etc.)
as intermediates for polymer photog. couplers are manufactured by hydrolysis of
benzoylaminopyrazolones II (R1, L = same as I; R2 = substituent; n = 0-5) in the presence of Ba compds. and alkali metal hydroxides, precipitation of the Ba
compds. as halides, and removal of the halides. Thus, II (R1 = 2,4,6-trichlorophenyl, R2 = H) was hydrolyzed in the presence of Ba(OH)2 and NaOH in MeOH, HCl added, filtered to remove BaCl2 and NaCl, and extracted
with PhMe to remove impurities. The residual aqueous solution was neutralized
with NaOH to give 70.5% I (R1 = 2,4,6-trichlorophenyl, R2 = H).
IT 112118-39-5 112118-41-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of aminopyrazolones by hydrolysis of benzoylaminopyrazolones in
the presence of Ba compds. and alkali metal hydroxides, and precipitation of
the Ba compds. as halides)
RN 112118-39-5 CAPLUS
CN Benzamide, N-[4-bromo-4,5-dihydro-5-oxo-1-(2,4,6-trichlorophenyl)-1H-

L4 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
pyrazol-3-yl]- (9CI) (CA INDEX NAME)



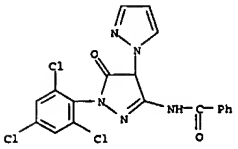
RN 112118-41-9 CAPLUS
CN Benzamide, N-[4',5'-dihydro-5'-oxo-1'-(2,4,6-trichlorophenyl)[1,4'-bi-1H-pyrazol]-3'-yl]- (9CI) (CA INDEX NAME)



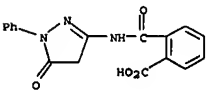
L4 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:900799 CAPLUS
DOCUMENT NUMBER: 138:4596
TITLE: Preparation of 3-amino-4-substituted-5-pyrazolones
INVENTOR(S): Suzuki, Akira; Yamakawa, Kazuyoshi
PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 14 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2002338548	A2	20021127	JP 2001-149314	20010518
PRIORITY APPLN. INFO.:			JP 2001-149314	20010518

OTHER SOURCE(S): CASREACT 138:4596; MARPAT 138:4596
AB The title compds., useful as intermediates for polymer couplers, etc., are prepared by hydrolyzing 4-substituted-5-pyrazolones containing (un)substituted benzoylamino group at 3-position with alkalis, e.g. Ba or Li compds. 3-Benzoylamino-4-(1-pyrazolyl)-1-(2,4,6-trichlorophenyl)-5-pyrazolone was treated with Ba(OH)2 in MeOH at 65° for 6 h to give 91.1% 3-amino-4-(1-pyrazolyl)-1-(2,4,6-trichlorophenyl)-5-pyrazolone (I). A photog. material containing a polymer coupler, prepared from I showed lower fog than a control material using polymer coupler derived from I prepared by acid hydrolysis.
IT 112118-41-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of 3-aminopyrazolones as intermediates for polymer couplers by alkali hydrolysis of N-benzoylamino derivs.)
RN 112118-41-9 CAPLUS
CN Benzamide, N-[4',5'-dihydro-5'-oxo-1'-(2,4,6-trichlorophenyl)[1,4'-bi-1H-pyrazol]-3'-yl]- (9CI) (CA INDEX NAME)



L4 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
yielded EtOCH2CONH2, needles from PhH, m. 80-2° (cf. Sommelet, Ann. chim. phys. [8] 9, 493). One mol. of EtOCH2COCH:NOH reacting with 1 mol. of o-C6H4(NH2)2 in 2 mols. of glacial AcOH gave rise to 2-ethoxymethylquinoxaline (H), CH:N.C6H4.N:CCH2OEt, b13 144°, neutral to litmus in aq. soln.; chloroplatinate, microcrystals, decomp. 250°; picrate, yellow powder, m. 216°. Upon gradual oxidation with alk. KMnO4, (A) yielded pyrazine-2,5,6-tricarboxylic acid, HO2CC:C(CO2H).N:CH.C(CO2H):N, silky needles, m. 191° (decompn.), isolated as the barium salt. The normal copper salt forms green microcrystals from aq. MeOH.
IT 860761-61-1, 5(4)-Pyrazolone, 3-(o-carboxybenzamido)-1-phenyl-
(preparation of)
RN 860761-61-1 CAPLUS
CN 5(4)-Pyrazolone, 3-(o-carboxybenzamido)-1-phenyl- (1CI) (CA INDEX NAME)



L4 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1915:15638 CAPLUS
DOCUMENT NUMBER: 9:15638
ORIGINAL REFERENCE NO.: 9:2517h-i,2518a-g
TITLE: Condensation of acid chlorides with the ethyl ester of (a) cyanoacetic acid, (b) malonic acid, and (c) acetoacetic acid. II. Experiments on ethyl γ-ethoxyacetoacetate
AUTHOR(S): Bradshaw, John; Stephen, Henry; Weizmann, Charles
CORPORATE SOURCE: Manchester
SOURCE: Journal of the Chemical Society, Transactions (1915), 107, 803-13
CODEN: JCHTA3; ISSN: 0368-1645
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.
AB cf. C. A. 8, 904. NaCH(CO2Et)2 reacting with o-C5H4(CO)2NHCH2COCl gave rise to ethyl bisphthaliminoacetylmalonate (A), [o-C6H4(CO)2NCH2CO]2C(CO2Et)2, needles, m. 176°. 1-Phenyl-3-phthaliminomethyl-5-pyrazolone, o-C6H4(CO)2NCH2.C:N.NPh.CO.CH2, microcrystals, m. 192° (decomposition), prepared from PhNHNH2 and Et phthaliminoacetoacetate, when hydrolyzed with alc. KOH yielded 1-phenyl-3-phthalaminomethyl-5-pyrazolone (B), yellow powder, m. 164° (decomposition). Et phthaliminoacetylmalonate (C) and PhNHNH2 condensed to form ethyl 1-phenyl-3-phthaliminomethyl-5-pyrazolone-4-carboxylate (D), o-C6H4(CO)2NHCH2C:N.NPh.CO.CHCO2Et, yellow powder, m. 215°, from which the corresponding (impure) phthalamino derivative was obtained. On fusion, the latter evolved CO2 and yielded (B). By warming an excess of PhNHNH2 with (A) in 50% AcOH, a mixture of (D) and phthaliminoacetylphenylhydrazide (E), o-C6H4(CO)2NCH2CONHNHPh, needles from MeOH, m. 199°, was obtained. (E) was readily formed by condensing o-C6H4(CO)2NCH2COCl with PhNHNH2. By treating (C) in KOH with NaNO2 and subsequently adding dilute H2SO4, α-hydroxyimino-γ-phthaliminoacetone, o-C6H4(CO)2NCH2CO.CH:NOH, prisms from PhH, m. 156° (decomposition), was obtained. When Et2NH was gradually added to an ice-cold mixture of 2 mols. EtOCH2COCH2CO2Et and 1 mol. AcH, ethyl ethylidenebis-γ-ethoxyacetoacetate, needles (from MeOH), m. 96°, was formed, which when heated for 20 hrs. with aqueous H2SO4, or preferably when dissolved in an equal volume of PhH and saturated with HCl, yielded 1-ethoxy-4-methyl-2-ethoxymethylcyclohexen-6-one, b14 157°, possessing a terpene-like odor; semicarbazone, plates, m. 232° (decomposition). EtOCH2COCHMeCO2Et (F), b16 115°, and EtOCH2COCHEtCO2Et (G), b15 124° (cf. Johnson, J. Chemical Society 35, 582), were formed by treating 1 mol. EtOCH2COCHNaCO2Et in EtOH with 1 mol. of MeI and EtI, resp. Similar reactions led to the formation of ethyl γ-ethoxy-α-propylacetoacetate, b18 137°; the corresponding α-isopropylacetoacetate, b18 131°, and α-isobutylacetoacetate, b10 128°, MeCH2COCH2OEt, b. 146°, and EtCH2COCH2OEt, b. 167° (cf. B.acte.ehal and Sommelet, Compt. rend. 138, 89), were obtained in poor yield from (F) and (G), resp., by heating the esters with H2O in sealed tubes at 210° for 1 hr. The other alkylacetoacetates were hydrolyzed in the same way, "acid hydrolysis" being the principal reaction as shown by the titration of the acid formed during the reaction. EtOCH2COCl and NH3 in dry Et2O

10797038 9/28/06

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